F 789 – Mecânica Quântica II

1º Semestre de 2023

12/04/2023

Aula 11

Aula passada

Teoria de Pauli:

a) C.C.O.C. agora contém operadores de spin que agem num espaço "interno":

$$\{X,Y,Z\} \to \{X,Y,Z,S^2,S_z\}$$
$$|\mathbf{r}\rangle \to |\mathbf{r},s,m\rangle$$
$$\{P_x,P_y,P_z\} \to \{P_x,P_y,P_z,S^2,S_z\}$$
$$|\mathbf{p}\rangle \to |\mathbf{p},s,m\rangle$$
$$m = -s,-s+1,\ldots,s-1,s$$

b) Para s=1/2, como o elétron: $s=1/2 \to |\mathbf{r},\varepsilon=\pm\rangle$ ou $|\mathbf{p},\varepsilon=\pm\rangle$

c) Ao momento angular de spin está associado um momento de dipolo magnético:

$$\mathbf{M} = 2\frac{\mu_B}{\hbar}\mathbf{S}$$

Aula passada

1. Espaço de estados $\mathcal{E}$

$$X\left|\mathbf{r},\varepsilon\right\rangle = x\left|\mathbf{r},\varepsilon\right\rangle$$
$$Y\left|\mathbf{r},\varepsilon\right\rangle = y\left|\mathbf{r},\varepsilon\right\rangle$$
$$Z\left|\mathbf{r},\varepsilon\right\rangle = z\left|\mathbf{r},\varepsilon\right\rangle$$
$$S^2\left|\mathbf{r},\varepsilon\right\rangle = \frac{3}{4}\hbar^2\left|\mathbf{r},\varepsilon\right\rangle$$
$$S_z\left|\mathbf{r},\varepsilon\right\rangle = \frac{\hbar}{2}\varepsilon\left|\mathbf{r},\varepsilon\right\rangle$$

$$\left\langle \mathbf{r}',\varepsilon' | \mathbf{r},\varepsilon\right\rangle = \delta_{\varepsilon,\varepsilon'}\delta^{(3)}\left(\mathbf{r}-\mathbf{r}'\right)$$ (ortonormalidade)

$$\sum_{\varepsilon}\int d^3r\left|\mathbf{r},\varepsilon\right\rangle\left\langle\mathbf{r},\varepsilon\right| = \mathbb{1}$$ (fechamento)

2. Representação $|\mathbf{r},\varepsilon>$

$$\left\langle \mathbf{r},\varepsilon|\psi\right\rangle = \psi_\varepsilon\left(\mathbf{r}\right) \to \left[\psi\right]\left(\mathbf{r}\right) = \begin{pmatrix} \psi_+\left(\mathbf{r}\right) \\ \psi_-\left(\mathbf{r}\right) \end{pmatrix}$$

$$\left\langle \psi|\mathbf{r},\varepsilon\right\rangle = \psi_\varepsilon^*\left(\mathbf{r}\right) \to \left[\psi\right]^\dagger\left(\mathbf{r}\right) = \begin{pmatrix} \psi_+^*\left(\mathbf{r}\right) & \psi_-^*\left(\mathbf{r}\right) \end{pmatrix}$$

$\boxed{\text{Spinores}}$

Aula passada

Produto escalar: $\langle \psi | \varphi \rangle = \int d^3r \left[\psi_+^* (\mathbf{r}) \varphi_+ (\mathbf{r}) + \psi_-^* (\mathbf{r}) \varphi_- (\mathbf{r}) \right]$

$$\langle \psi | \psi \rangle = \int d^3r \left[\left| \psi_+ (\mathbf{r}) \right|^2 + \left| \psi_- (\mathbf{r}) \right|^2 \right]$$

3. Operadores: levam spinores em spinores (linearmente)

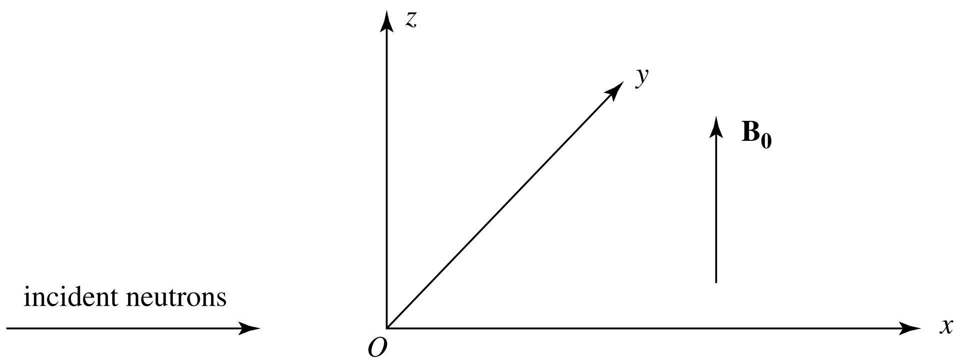
$$[\psi'] (\mathbf{r}) = [\![A]\!] [\psi] (\mathbf{r})$$

$[\![A]\!]$ tem tanto estrutura matricial (espaço de spin) quanto opera na parte orbital.

Exemplos: $[\![\mathbf{S}]\!] = \frac{\hbar}{2} \boldsymbol{\sigma}$ $\qquad [\![\mathbf{P}]\!] = \mathbb{1} \frac{\hbar}{i} \nabla$

$$[\![\mathbf{S} \cdot \mathbf{P}]\!] = \frac{\hbar}{2} \frac{\hbar}{i} \begin{pmatrix} \frac{\partial}{\partial z} & \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} & -\frac{\partial}{\partial z} \end{pmatrix}$$

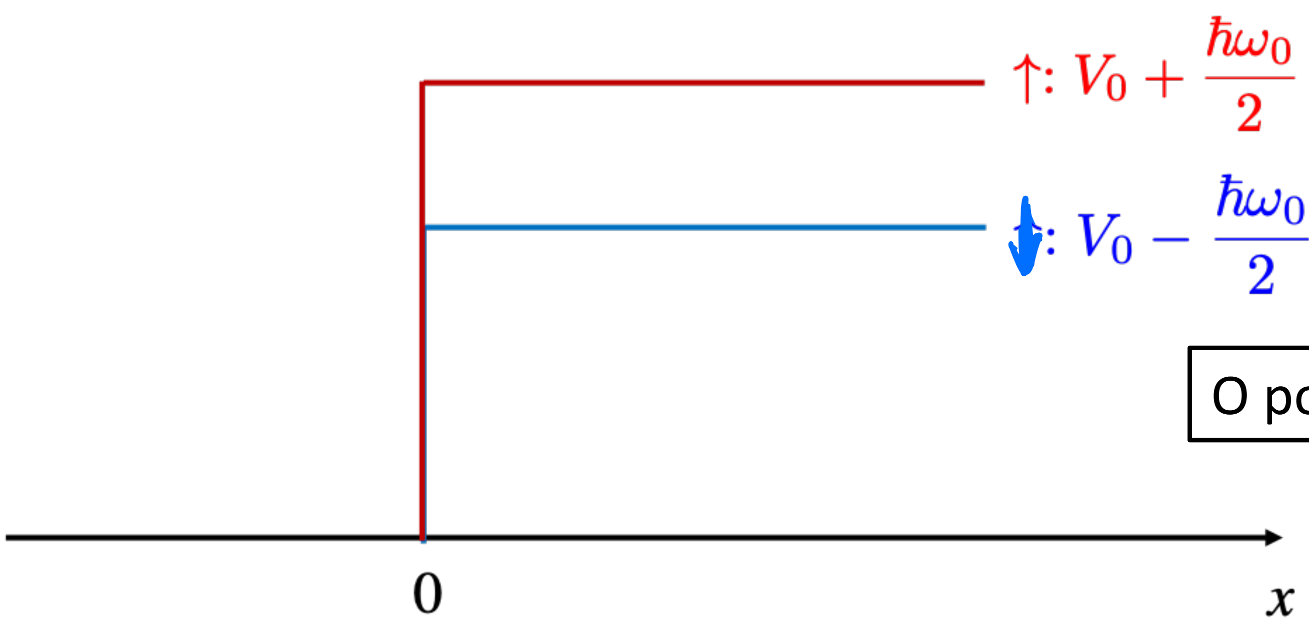
Exemplo: feixe de nêutrons incidente num ferromagneto



$$V(x) = \begin{cases} 0 & x < 0, \\ V_0 + \omega_0 S_z & x > 0. \end{cases}$$

$$\omega_0 = -\gamma B_0$$

$$-\vec{\mu}\cdot\vec{B} = -\gamma B_0 S_z$$



O potencial depende do spin.

$$[\psi](x) = \begin{pmatrix} A_+ e^{ikx} + B_+ e^{-ikx} \\ A_- e^{ikx} + B_- e^{-ikx} \end{pmatrix} \quad k = \frac{\sqrt{2mE}}{\hbar} \quad (x<0)$$

$$E = \frac{\hbar^2 k^2}{2m}$$

$$A e^{ikx} + B e^{-ikx}$$

a) $E > V_0 + \frac{\hbar\omega_0}{2}$

$$[\psi](x) = \begin{pmatrix} C_+ e^{ik'_+ x} \\ C_- e^{ik'_- x} \end{pmatrix} \quad (x>0)$$

$\uparrow$: $\left[\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \left(V_0 + \frac{\hbar\omega_0}{2}\right)\right]\psi_+(x) = \frac{\hbar^2 k^2}{2m}\psi_+(x) \Rightarrow k'_+ = \frac{\sqrt{2m\left(E - V_0 - \frac{\hbar\omega_0}{2}\right)}}{\hbar}$

$\downarrow$: $\longrightarrow$ $k'_- = \frac{\sqrt{2m\left(E - V_0 + \frac{\hbar\omega_0}{2}\right)}}{\hbar}$

b) $E < V_0 - \frac{\hbar\omega_0}{2}$:

$$[\psi](x) = \begin{pmatrix} D_+ e^{-\rho_+ x} \\ D_- e^{-\rho_- x} \end{pmatrix} \quad (x>0) \qquad \rho_\pm = \frac{\sqrt{2m\left(V_0 \pm \frac{\hbar\omega_0}{2} - E\right)}}{\hbar}$$

ρ : $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \left(V_0 + \frac{\hbar\omega_0}{2}\right)\right]\psi_+(x) = E\,\psi_+(x)$

$$\frac{d^2}{dx^2}\psi_+(x) = \frac{2m}{\hbar^2}\underbrace{\left(V_0 + \frac{\hbar\omega_0}{2} - E\right)}_{>0}\psi_+(x) \equiv \rho_+^2\,\psi_+(x)$$

c) $V_0 - \frac{\hbar\omega_0}{2} < E < V_0 + \frac{\hbar\omega_0}{2}$

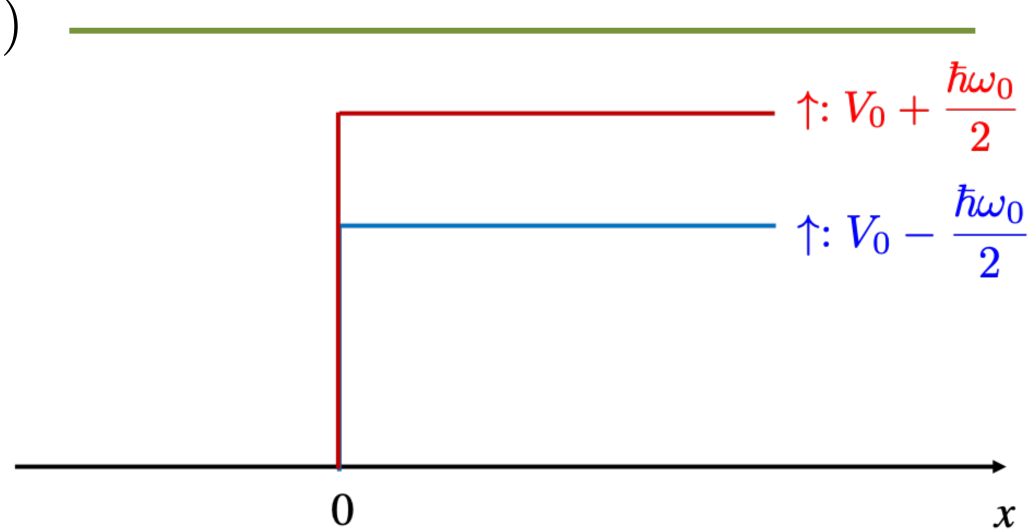
$$[\psi](x) = \begin{pmatrix} D_+ e^{-\rho_+ x} \\ C_- e^{ik'_- x} \end{pmatrix} \quad (x>0)$$

$\Rightarrow$ PRÓXIMO PASSO: IMPOR EM $x=0$ A CONTINUIDADE DE $[\psi](x)$ E $\frac{d}{dx}[\psi](x)$

CASO a)

$$[\psi](x) = \begin{pmatrix} A_+ e^{ikx} + B_+ e^{-ikx} \\ A_- e^{ikx} + B_- e^{-ikx} \end{pmatrix} \quad (x < 0)$$

$(E > V_0 + \hbar\omega_0/2)$

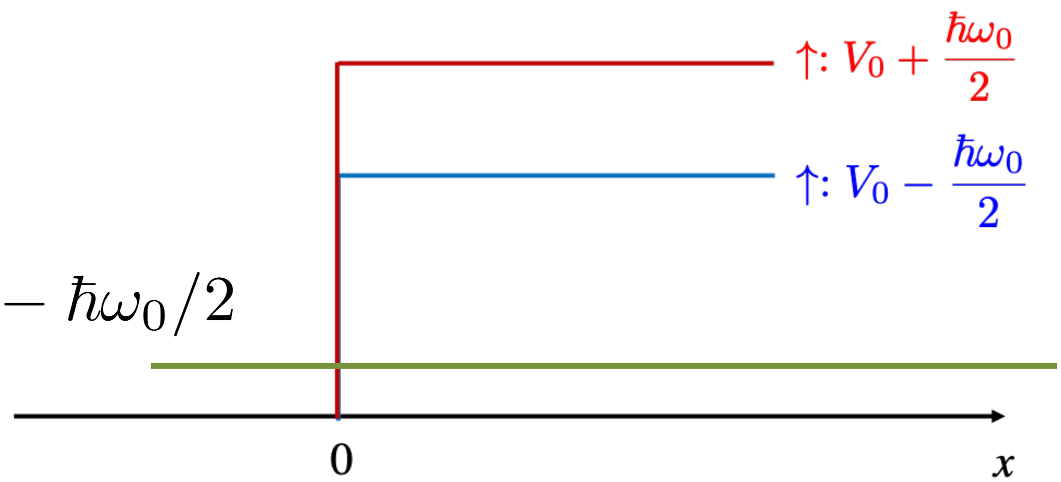


$$(a)\ [\psi](x) = \begin{pmatrix} C_+ e^{ik'_+ x} \\ C_- e^{ik'_- x} \end{pmatrix} \quad (x > 0) \qquad k'_\pm = \frac{\sqrt{2m\left(E - V_0 \mp \hbar\omega_0/2\right)}}{\hbar}$$

CASO b)

$$[\psi](x) = \begin{pmatrix} A_+ e^{ikx} + B_+ e^{-ikx} \\ A_- e^{ikx} + B_- e^{-ikx} \end{pmatrix} \quad (x < 0)$$

$E < V_0 - \hbar\omega_0/2$

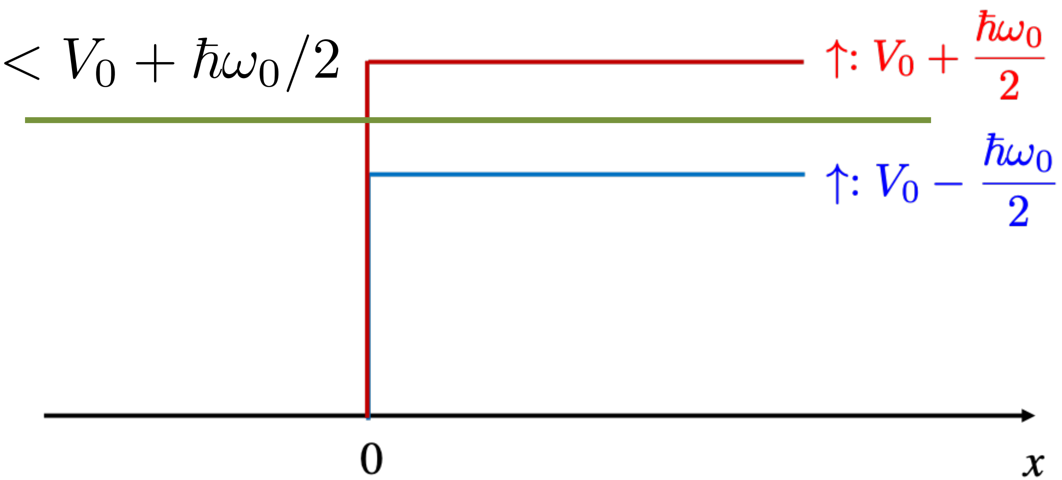


$$(b)\ [\psi](x) = \begin{pmatrix} D_+ e^{-\rho'_+ x} \\ D_- e^{-\rho'_- x} \end{pmatrix} \quad (x > 0) \qquad \rho_\pm = \frac{\sqrt{2m\,(V_0 \pm \hbar\omega_0/2 - E)}}{\hbar}$$

CASO c)

$$[\psi](x) = \begin{pmatrix} A_+ e^{ikx} + B_+ e^{-ikx} \\ A_- e^{ikx} + B_- e^{-ikx} \end{pmatrix} \; (x < 0)$$

$$V_0 - \hbar\omega_0/2 < E < V_0 + \hbar\omega_0/2$$



$$(c)\; [\psi](x) = \begin{pmatrix} D_+ e^{-\rho'_+ x} \\ C_- e^{ik'_- x} \end{pmatrix} \; (x > 0)$$

Resultado de "casar" as funções de onda

COEF. REFLEXÃO

COEF. TRANSMISSÃO $\left(\times \frac{k'_\pm}{k}\right)$

Caso (a):
$$\frac{B_\pm}{A_\pm} = \frac{k - k'_\pm}{k + k'_\pm}, \quad \frac{C_\pm}{A_\pm} = \frac{2k}{k + k'_\pm}$$

Caso (b):
$$\frac{B_\pm}{A_\pm} = \frac{k - i\rho_\pm}{k + i\rho_\pm}, \quad \frac{D_\pm}{A_\pm} = \frac{2k}{k + i\rho_\pm}$$

Caso (c):
$$\frac{B_+}{A_+} = \frac{k - i\rho_+}{k + i\rho_+}, \quad \frac{D_+}{A_+} = \frac{2k}{k + i\rho_+}$$
$$\frac{B_-}{A_-} = \frac{k - k'_-}{k + k'_-}, \quad \frac{C_-}{A_-} = \frac{2k}{k + k'_-}$$

OLHANDO APENAS O COEF. DE REFLEXÃO DO CASO (C)

$$R_+ = \left|\frac{B_+}{A_+}\right|^2 = \left|\frac{k - i q_+}{k + i q_+}\right|^2 = \frac{|k - i q_+|^2}{|k + i q_+|^2} = 1$$

$$R_- = \left|\frac{B_-}{A_-}\right|^2 = \left|\frac{k - k'_-}{k + k'_-}\right|^2 < 1$$

$\Rightarrow$ REFLEXÃO TOTAL DOS NÊUTRONS COM SPIN $\uparrow$

" PARCIAL " " " " $\downarrow$

Polarização do feixe refletido

Suponha que o feixe incidente é não polarizado: o elétron tem probabilidade ½ de ser up e ½ de ser down. Qual é a polarização do feixe refletido?

FEIXE INCIDENTE NÃO POLARIZADO: $N_+ = N_- =$ NÚMERO DE NÊUTRONS INCIDENTES

FEIXE REFLETIDO:

$N^R_+ = R_+ N_+ = N_+$ $\qquad N^R_- = R_- N_- < N_-$

POLARIZAÇÃO: $P = \frac{|N_+ - N_-|}{N_+ + N_-}$; $P_{INC} = 0$

$N_+ = N$

$$P_{REF} = \frac{N^R_+ - N^R_-}{N^R_+ + N^R_-} = \frac{N_+ - R_- N_-}{N_+ + R_- N_-} = \frac{1 - R_-}{1 + R_+}$$

UM NÊUTRON COM SPIN NA DIREÇÃO X!

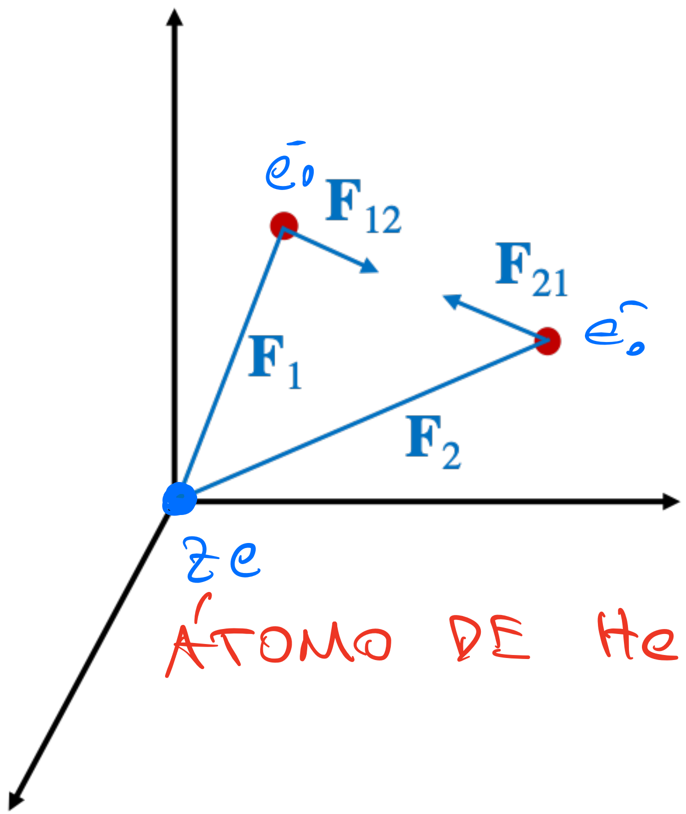
$$|+\rangle_x = \frac{1}{\sqrt{2}}\left[|+\rangle + |-\rangle\right]$$

O QUE ACONTECE COM OS FEIXES REFLETIDO E TRANSMITIDO?

O SPIN MÉDIO GIRA DE DIREÇÃO DEPENDENDO DA ENERGIA DO FEIXE INCIDENTE.

Adição de momentos angulares

O problema



2 momentos angulares: não há conservação separada de cada um deles, mas o momento angular total é conservado. COMO UM ÁTOMO DE 2 e^-'s

$$H = H_1 + H_2 + H_{12}$$

$$H_1 = \frac{\vec{P}_1^{\,2}}{2m} + V(\vec{R}_1) \qquad H_2 = \frac{\vec{P}_2^{\,2}}{2m} + V(\vec{R}_2)$$

$$V(\vec{R}) = -\frac{Ze^2}{R}$$

$$H_{12} = v(|\vec{R}_1 - \vec{R}_2|) = \frac{e^2}{|\vec{R}_1 - \vec{R}_2|}$$

JÁ VIMOS QUE:

$$[H_1, \vec{L}_1] = [H_2, \vec{L}_2] = 0$$

ONDE $\vec{L}_{1,2}$ = MOMENTO ANGULAR ORBITAL DO e^-s 1,2

CLARO QUE: $[H_1, \vec{L}_2] = 0 = [H_2, \vec{L}_1]$

$\Rightarrow [H_1, \vec{L}_1 + \vec{L}_2] = 0$ E $[H_2, \vec{L}_1 + \vec{L}_2] = 0$

ENTRETANTO: $[H_{12}, \vec{L}_1] \neq 0$ E $[H_{12}, \vec{L}_2] \neq 0$

MAS, COMO VEREMOS, $[H_{12}, \vec{L}_1 + \vec{L}_2] = 0$!

PROVA:

$$[L_{1z}, H_{12}] = [(X_1 P_{1y} - Y_1 P_{1x}), \vartheta(|\vec{R}_1 - \vec{R}_2|)] = (*)$$

ABRINDO O COMUTADOR:

$$(*) = \frac{\hbar}{i}\left(x_1 \frac{\partial \vartheta}{\partial y_1} - y_1 \frac{\partial \vartheta}{\partial x_1}\right) \neq 0$$

$$[L_{2z}, H_{12}] = \frac{\hbar}{i}\left(x_2 \frac{\partial \vartheta}{\partial y_2} - y_2 \frac{\partial \vartheta}{\partial x_2}\right) \neq 0$$

$$[x p_x, f(x)]\psi(x) = \frac{\hbar}{i}\left[x\frac{\partial}{\partial x}(f\psi) - f\, x\frac{\partial}{\partial x}(\psi)\right]$$

$$\frac{\hbar}{i}\, x\frac{\partial}{\partial x}$$

$$= \frac{\hbar}{i}\left[x f'\psi + \cancel{x f\psi'} - \cancel{f x\psi'}\right]$$

$$= \frac{\hbar}{i}\left[x\frac{\partial f}{\partial x}\right]\psi$$

$$x_1\frac{\partial v}{\partial y_2} + x_2\frac{\partial v}{\partial y_2} = \left[\frac{-x_1(y_1-y_2)}{[\quad]^{1/2}} + \frac{x_2(y_1-y_2)}{[\quad]^{1/2}}\right] v'$$

$$\frac{\partial v}{\partial y_2} = \frac{\partial}{\partial y_2} v(|\vec{r}_1-\vec{r}_2|) = \frac{\partial}{\partial y_2} v\left(\left[(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2\right]^{1/2}\right)$$

$$= v'\,\frac{(y_1-y_2)(-1)}{[\quad]^{1/2}}$$

$$\frac{\partial v}{\partial y_1} = v'\,\frac{(y_1-y_2)}{[\quad]^{1/2}}$$

$$x_2 \frac{\partial v}{\partial y_2} - y_2 \frac{\partial v}{\partial x_2} = \frac{v'}{[\ ]^{1/2}} \left[x_2 (y_2 - y_1) - y_2 (x_2 - x_1) \right]$$

AO FINAL:

$$[L_{1z} + L_{2z}, H_{12}] = \frac{\hbar}{i} \frac{v'}{[\ ]^{1/2}} \cdot \Big[x_1 (y_1 - y_2) - y_1 (x_1 - x_2)$$

$$+ x_2 (y_2 - y_1) - y_2 (x_2 - x_1) \Big] = 0$$

ANALOGAMENTE PARA $L_{1x} + L_{2x}$ E $L_{1y} + L_{2y}$

$$\Rightarrow [\vec{L}_1 + \vec{L}_2, H_{12}] = 0$$

$$[\vec{L}_1 + \vec{L}_2, H] = 0$$